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SMOOTH PARTICLE HYDRODYNAMICS FOR GRAIN SCALE MULTI-PHASE FLUID SIMULATIONS

DAVID W. HOLMES*, JOHN R. WILLIAMS* AND PETER TILKE†

*Civil and Environmental Engineering
Massachusetts Institute of Technology
77 Massachusetts Avenue, Cambridge, MA 02139-4307, US
e-mail: dholmes@mit.edu, web page: http://www.mit.edu/

†Department of Mathematics and Modeling
Schlumberger-Doll Research Center
1 Hampshire Street, Cambridge, MA 02139-1578, US

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Abstract. In this paper, the implementation of a 3D smooth particle hydrodynamics (SPH) simulator is presented. The method can simulate multiple fluid phases and is capable of reproducing complex phase interface phenomena such as surface tension, contact angle and wettability. After a brief development, we present on simulation results from several industrially relevant examples including 3D multi-phase flows in granular media.

1 INTRODUCTION

Complex gas/liquid/solid interactions are of interest in many areas of geoscience including enhanced oil recovery (EOR), groundwater contamination, carbon sequestration and hydrates mining. Such interactions have particular importance at the grain scale where phase interfacial physics such as capillary forces, can dictate much of the dynamics of a highly confined system. A significant amount of insight can be gained by accurately simulating multi-phase fluid flows at such scales, however, this has been a challenging area for existing numerical methods to address.

Smooth particle hydrodynamics (SPH) is a meshfree Lagrangian particle method first proposed for astrophysical problems which is now finding increasing application in the area of fluid mechanics, particularly for problems dominated by multi-phase and/or multi-physics phenomena[1;2]. SPH is ideally suited to the simulation of such systems due to it's updated Lagrangian and particle based nature. By advecting mass with each particle, phase interfaces between different fluids are defined intrinsically. Additionally, by the inclusion of additional pair-wise inter-particle forces[2], surface tension can be accounted for via a direct analog to the actual molecular mechanisms which drive such phenomena in reality. This allows SPH to easily account for complex behaviors related to solid/liquid contact angle and surface wettability.

In this work it has been our aim to develop a numerical simulator to model grain scale phenomena related to the recovery of oil from ground rock. An SPH simulator has been developed for this purpose and the fundamentals behind the multi-phase and surface tension components of the simulator will be of particular focus in this paper. From an industrial standpoint, a key advantage of this SPH simulator is in its ability to allow numerical experimentation, for example, testing the effect that different surfactants and water invasion techniques have on oil recovery. In this way new EOR techniques can be developed. Several example problems are presented which illustrate such tests.

2 METHODOLOGY

SPH theory has been detailed widely in the literature with various formulations having been proposed. The methodology of authors such as Tartakovsky and Meakin[2;3] and Hu and Adams[1] has been shown to perform well for the case of multi-phase fluid flows. Their *particle number density* variant of the conventional SPH formulation removes erroneous artificial surface tension effects between phases and allows for phases of significantly differing densities. Such a method has been used in this work.

The discretized particle number density SPH equations for some field quantity, A_i, and its gradient are given as

$$A_i = \sum_j \frac{A_j}{n_j} W\left(\boldsymbol{r}_i - \boldsymbol{r}_j, h\right), \qquad \nabla A_i = \sum_j \frac{A_j}{n_j} \nabla_i W\left(\boldsymbol{r}_i - \boldsymbol{r}_j, h\right) \tag{1}$$

where $n_i = \rho_i / m_i = \sum_j W\left(\boldsymbol{r}_i - \boldsymbol{r}_j, h\right)$ is the particle number density term, while W is the smoothing function (typically a gaussian or some form of spline), h is the smoothing length and $\boldsymbol{r}$ are position vectors. These expressions are applied to the Navier-Stokes conservation equations to determine the SPH equations of motion.

Computing density directly from $(1)_a$, gives

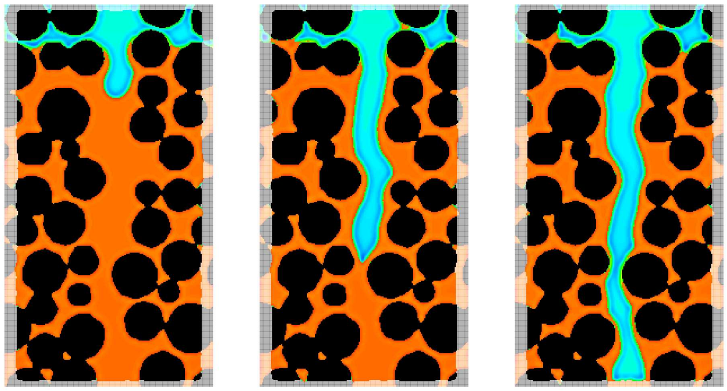
$$\rho_i = m_i \sum_j W\left(\boldsymbol{r}_i - \boldsymbol{r}_j, h\right) \tag{2}$$

where this expression conserves mass exactly, much like the summation density approach of conventional SPH.

An appropriate term for particle velocity rate has been provided by Morris et al[4], and used by Tartakovsky and Meakin[3], where

$$\frac{d\boldsymbol{\nu}_i}{dt} = -\frac{1}{m_i} \sum_{j=1}^{N} \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \frac{\partial W_{ij}}{\partial \boldsymbol{r}_i} + \frac{1}{m_i} \sum_{j=1}^{N} \frac{(\mu_i + \mu_j)}{n_i n_j} \left(\boldsymbol{v}_i - \boldsymbol{v}_j\right) \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|^2} \cdot \frac{\partial W_{ij}}{\partial \boldsymbol{r}_i} + \boldsymbol{F}_i \tag{3}$$

and where P_i is particle pressure, μ_i is the dynamic viscosity, $\boldsymbol{v}_i$ is the particle velocity and $\boldsymbol{F}_i$ is the body force applied on the i^{th} particle.



$t = 150$ $t = 710$ $t = 1000$

Figure 1: Simulation results for water invasion experiment where water (top fluid) is a non-wetting phase, displacing oil (bottom fluid) which is a wetting phase. Grain geometry from[2].

Surface tension is introduced into the method via the superimposition of pair-wise inter-particle forces following Tartakovsky and Meakin[2]

$$\boldsymbol{F}_{ij} = \begin{cases} s_{ij} \cos\left(\frac{1.5\pi}{\kappa h} |\boldsymbol{r}_j - \boldsymbol{r}_i|\right) \frac{\boldsymbol{r}_j - \boldsymbol{r}_i}{|\boldsymbol{r}_j - \boldsymbol{r}_i|} & |\boldsymbol{r}_j - \boldsymbol{r}_i| \leq \kappa h \\ 0 & |\boldsymbol{r}_j - \boldsymbol{r}_i| > \kappa h \end{cases} \tag{4}$$

where s_{ij} is the strength of force between particles i and j, while κh is the interaction distance of a particle. By defining s_{ij} as being stronger between particles of the same phase, than between particles of a different phase, surface tension comes out naturally as a result of force imbalances at phase interfaces. Similarly, s_{ij} can be defined to control the wettability properties of a solid.

To facilitate the simulation of complex pore geometries in three-dimensions, the developed SPH simulator has been implemented within a parallel numerical framework developed elsewhere. Results showing the performance of the code for grain scale multi-phase fluid simulations are presented in what follows.

3 RESULTS

Numerical experiments were carried out on the effect of wettability on oil recovery for water invasion through idealized porous media in two- and three-dimensions. Fig's. 1 and 2 show results for two-dimensional tests where grains were initially surrounded by oil and were invaded with water from the top surface. In each figure, images are provided for three representative times from the simulation. Model geometry is a reproduction of that of Tartakovsky and Meakin[2]. From the figures it is clear that, where water is assigned as the wetting phase (Fig. 2), a much greater amount of oil is removed from the system. These results agree well with those of Tartakovsky and Meakin for the same problem.

Fig. 3 shows an equivalent numerical experiment in three-dimensions, again, with water invading oil filled pores from the top surface. With a relatively high porosity, it is evident

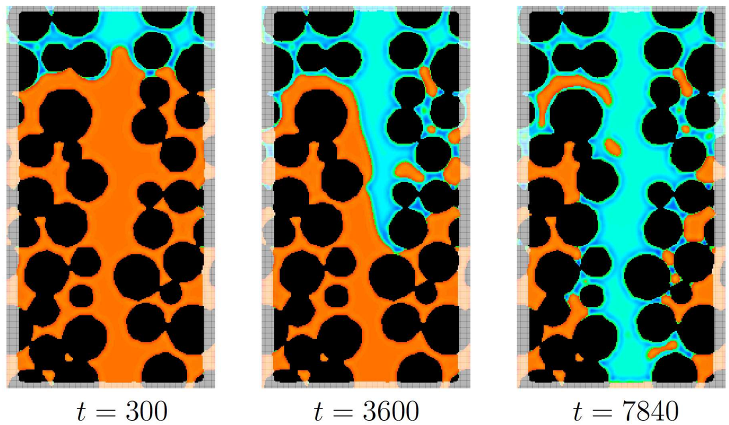


Figure 2: Simulation results for water invasion experiment where water (top fluid) is a wetting phase, displacing oil (bottom fluid) which is a non-wetting phase. Grain geometry from [2].

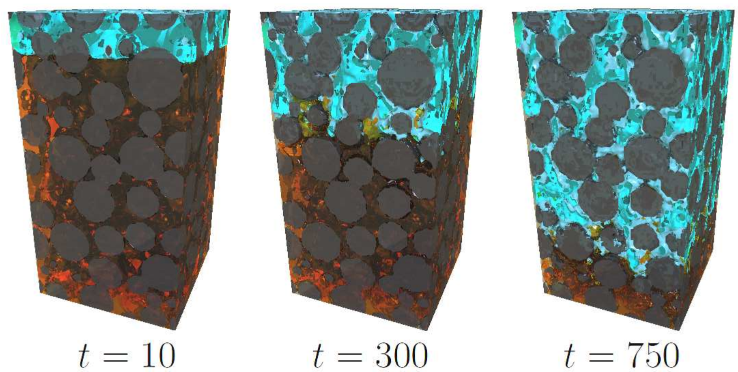


Figure 3: 3D water invasion experiment results where a wetting water phase (top fluid) invades and washes out a non-wetting oil phase (bottom fluid) through a random packing of spherical grains.

that the majority of the oil is removed from the grains. We are currently conducting similar testing on lower porosity systems.

References

[1] X. Y. Hu and N. A. Adams, A multi-phase SPH method for macroscopic and mesoscopic flows. *Journal of Computational Physics*, **213**, 844–861 (2006).

[2] A. M. Tartakovsky and P. Meakin, Pore scale modeling of immiscible and miscible fluid flows using smoothed particle hydrodynamics. *Advances in Water Resources*, **29**, 1464–1478 (2006).

[3] A. M. Tartakovsky and P. Meakin, A smoothed particle hydrodynamics model for miscible flow in three-dimensional fractures and the two-dimensional rayleigh-taylor instability. *Journal of Computational Physics*, **207**, 610–624 (2005).

[4] J. P. Morris, P. J. Fox and Y. Zhu, Modeling low Reynolds number incompressible flows using SPH. *Journal of Computational Physics*, **136**, 214–226 (1997).